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Optical properties and structure of Si/InAs/Si layers grown by MBE on Si substrate

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Abstract. Epitaxial Si/InAs/Si heterostructure grown on (001) Si substrate by molecular beam epitaxy (MBE) and annealed at 800°C was investigated by High Resolution Transmission Electron Microscopy (HRTEM). Extensive interdiffusion leads to the formation of an InAs solid solution in the Si cap layer. Additionally, InAs-enriched regions with extensions of 6 nm, which exhibit two kinds of ordering are observed. The ordering of InAs molecules has occurred. The sample show photoluminescence in the 1.3 μm region, which is tentatively attributed to the recombination of excitons localised in the ordered regions.

Introduction

The potential benefit from combining the advantageous optical properties and flexibility of III–V semiconductors with silicon technology widely used in microelectronics has attracted great interest for decades. Up to now, researchers have focussed on the growth of continuous layers of III–V materials on silicon [1]. The large misfit between Si and, e.g., InAs ($\varepsilon = 10.6\%$) renders the growth of electronic or optical quality material practically unresolvable problem. More recently, the possibility to exploit the formation of narrow-gap III–V islands on Si substrates has been pointed out [2]. Indeed, such small InAs islands on Si(100) surface have been observed by scanning tunnelling microscopy and high-resolution transmission electron microscopy (HRTEM) [3, 4]. HRTEM investigations of capped InAs/Si structures revealed a high density of coherent InAs clusters with typical dimensions in the 3 nm region at the InAs/Si interface for optimised growth conditions [5, 6]. Such samples exhibit a broad photoluminescence (PL) peak in the 1.3 μm region at 10 K [3]. Detailed optical investigations of this PL line indicated a k-indirect type II transition, which has been tentatively attributed to excitons localised in the small coherent InAs clusters [7]. The extreme small size (< 3 nm) of these clusters might, however, prevent sufficient carrier localisation. The present work present a detailed structural characterisation of such InAs-Si layers providing new insight into the origin of the 1.3 μm PL peak

Experimental

The InAs/Si heterostructure was grown by molecular beam epitaxy (MBE) on p-type Si(100) substrate using an EP 1203 machine. The growth rates for InAs and Si were 0.03 nm/s and 0.017 nm/s, respectively, and the As/In flux ratio was ∼ 4. InAs was deposited at a substrate temperature of $T_s = 350^\circ\text{C}$. The nominal thickness of the deposited InAs was 1.6 ML. Immediately after the InAs deposition, a 10 nm Si cap layer was grown at the

same $T_s = 350^\circ\text{C}$ followed by a 10 min annealing step at 700°C . Further 40 nm Si cap layer was grown at 700°C with a final 10 min annealing step at 800°C to smooth resulting surface. The crystalline quality of the structure and the composition of the grown layers were investigated by techniques of transmission electron microscopy (TEM). PL spectra were measured at a temperature of 7K using Argon laser excitation.

Results

Typical cross-section and plan-view images of the investigated structure are shown in Fig. 1(a,b) respectively. The plan-view image shows the good structural quality of the sample with a relatively low density (10^8 1/cm^2) of structural defects, marked A in Fig. 1(b). These defects (A) are located at the InAs/Si interface and do not penetrate into Si cap layer. First, the average InAs concentration in the Si cap layer can be estimated from selected area diffraction (SAD) taken at once from substrate and cap layer in cross-sections sample as shown in Fig. 1(a). Such SAD pattern reveal a splitting of reflections in [001] direction perpendicular to the layer surface (Fig. 1(c)). This splitting is attributed to a tetragonal distortion of Si cap layer due to the formation of an InAs solid solution. The magnitude of the observed splitting of the reflection (206) measured in SAD corresponds to a tetragonal distortion $\Delta = \Delta g/g_{(206)} = \Delta a/a_{\text{Si}} = 0.007$. The volume of the distorted unit cell is $V_t = a_{\text{Si}}(1 + \Delta a/a_{\text{Si}})^{1/3}$. It immediately follows that average cubic unit cell parameter of

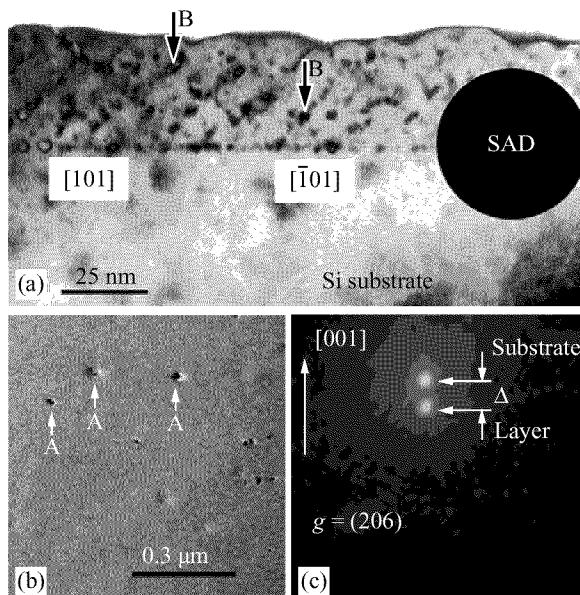


Fig. 1. (a) [010] cross section TEM image. Ordered InAs regions are marked as B. Black circle SAD indicate the region from what the Selected Area Diffraction was taken. (b) Plan view [001] TEM image. Defects marked as A in are situated at the interface. (c) Selected Area Diffraction (SAD) from cross section sample. Diffraction was taken from the region marked by black circle in (a). Sample was oriented along [010]. $\Delta = \Delta g/g_{(206)}$, $g = (206)$ diffraction vector, Δg the change in g .

the solid solution a_{ss} is given by:

$$a_{ss} = V_t^{1/3} = a_{\text{Si}}(1 + \Delta a/a_{\text{Si}})^{1/3}. \quad (1)$$

Taking a_{ss} as to be linearly dependent on the InAs concentration in the Si matrix, it follows:

$$C_{\text{InAs}} = (a_{ss} - a_{\text{Si}})/(a_{\text{InAs}} - a_{\text{Si}}) \quad (2)$$

where C_{InAs} —concentration of InAs in Si cap layer, a_{Si} , a_{InAs} —unit cell parameters of Si and InAs respectively. Substitution of $\Delta a/a_{\text{Si}} = 0.007$ into Eqs. (1), (2) gives $C_{\text{InAs}} = 0.004$. Thus the averaged composition of the cap layer can be written as $\text{Si}_{0.996}(\text{InAs})_{0.004}$.

Second, in high resolution cross-sectional images the dark regions marked by B in Fig. 1(a) reveal a doubling of periodicity of $\{002\}$ lattice planes (Fig. 2(a)). It leads to appearance of diffuse maxima situated halfway between $\pm(202)$ matrix reflections in the Fourier transformed image (FFT) (see insert in Fig. 2(a)). This result can be interpreted as a partial ordering of InAs in Si. A possible idealised model of such an ordering is shown in Fig. 2(b) where InAs occupies every other atomic (101) plane inclined by 45° to the surface. A HREM image (Fig. 2(c)) simulated on the basis of this structural model shows that the darker rows correspond to InAs atomic rows. It is obvious that the contrast calculated for an ideal ordering is in a qualitative agreement with the experimental image. These partially ordered regions can also be observed at low magnification using diffraction contrast technique (see features B in Fig. 1(a)). In this case, the image contrast (dark regions) results from variations of the extinction distance. The size of coherent ordered regions (≥ 6 nm) is about 2 times larger than the size of coherent InAs clusters formed at the InAs/Si interface described in a former paper [5].

Figure 3 depicts a low temperature PL spectrum of the investigated sample revealing a broad PL peak in the $1.3 \mu\text{m}$ region. Recently, this luminescence has been studied in detail in a different sample, suggesting a k-indirect type II transition in the epitaxial layer [7]. Such a transition is indeed expected for coherent InAs clusters observed near the InAs/Si interface. However, the small size (~ 3 nm) of such clusters might be too small for sufficient carrier localisation. As shown above, the Si-cap layer is actually a Si-InAs solid solution with ordered InAs-rich regions. The ordered regions with a high InAs concentration (and therefore smaller band gap) and a size of ~ 6 nm, can provide sufficient carrier localization to explain the observed $1.3 \mu\text{m}$ emission. The incorporation of InAs molecules into the Si

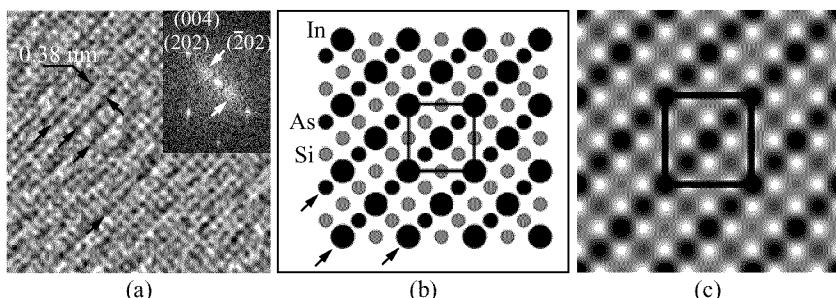


Fig. 2. (a) [010] cross section HRTEM image. Doubled periodicity 0.38 nm is marked. Fourier transformation of the image is inserted in upper right corner. Diffuse maxima on the halfway between central beam and $\pm(202)$ reflections indicate to the ordering. (b) Idealised model of ordering. (c) Theoretical image calculated according to the model in (b). Unit cell is outlined.

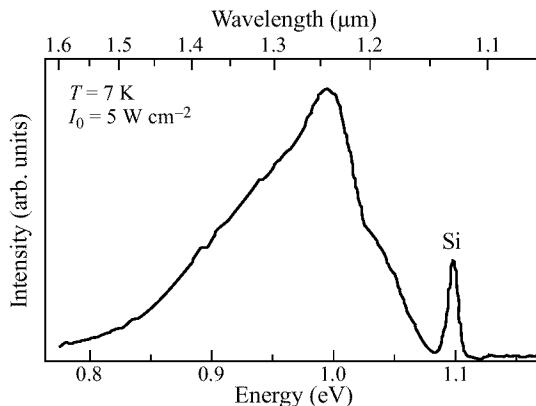


Fig. 3. PL spectrum of the investigated sample showing a broad luminescence at $1.25 \mu\text{m}$. The peak at $1.1 \mu\text{m}$ correlates to emission from the Si bulk.

is expected to shift the relative positions of the conduction and valence bands leading to a quantum structure.

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